INTRODUCTION TO
COMPUTATIONAL BIOLOGY

BS M123, BME 195, CS 183, MB 223, BME 295

Bren Hall - DBH 1500
TuTh 11:00am -12:15pm

Ray Luo, Ph.D. MBB/BME
Email: ray.luo@uci.edu
Tel: x4-9528
Office hours: by appointment at NSI 3206/3144

TA: Jeff Holden
Email: holdenj@uci.edu

Syllabus

This is an introduction to structural molecular biology using computational methods. Besides providing a fundamental background in biochemistry and molecular biology, it also surveys a wide variety of applications to the current biomedical research fields. Its aim is to give an understanding of the biological problems that arise and how computational methods are developed to address them. It does not train students to be expert users of specific methods, but train students to appreciate the basic ideas of the methods and how the methods are used in the analysis of biomedical questions.

Student involvement in the classroom is an integral component for this course. Successful completion of the course will benefit students in the following crucial areas that are often overlooked in other classes on campus: (a) development of skills to summarize and critique formal research reports; (b) development of abilities to prepare and present a scholarly subject professionally in front of a large audience.

Prerequisite

Willing to think quantitatively in biology, i.e. comfortable with college math,
phys, and chem.

**Grading Policy**

Grade will be based on literature presentation and literature critique starting tentatively on Oct 18.

- Literature presentation, 65%, is a formal presentation of an assigned journal paper. Presentation is set to be 17 min (about 16 slides) and 8 min of questions. Please follow your summary outlines (see below) to prepare your presentations. Also remember to introduce the PI’s group and research interests before your paper presentation to make it more interesting. The time limit will be enforced. You will lose points if your talk is either too short (less than 15 min) or too long (over 20 min).

The student presentations will be given by either one graduate student or two undergraduate students. If one of the undergraduates drops off the class, the remaining student will automatically receive a bonus one-tick higher letter grade for presenting alone. The plan is for the students to start presentations on Oct 18. I will assign graduate students to present first. These will be followed by presentations by undergraduates so you have a better idea how to present.

Past experiences show that we can only arrange two student presentations per lecture due to the long discussion and question time after each talk. Thus the class will be divided into four groups (up to 12 students per group) for easy management. The group division will be posted on Oct 9 when the enrollment starts to stabilize.

- Literature critique, 35%, is a weekly summary of an article assigned for your reading. If your group members are presenting on that day, you will be assigned to read the same paper to be presented. If there is no student presentation on a specific date, you will be assigned to read a paper to be emailed one week ahead of time. This happens when we have an outside lecturer giving a formal seminar (see below). The students who are presenting that week are exempt from this assignment. We will ensure that each student reviews the same number of papers by the end of the quarter.

The summary should highlight the following. (1) What is the biomedical
significance of the research? (2) What is the specific question to be answered in the research? (3) How does the author approach the question? (4) What is the conclusion? (5) What is the scope or limitation of the conclusion? Use no more than 250 words in your summary. Also, prepare two questions that you can potentially ask the presenter(s).

- Classroom involvement in strongly encouraged. For each student presentation, every other student in the class is encouraged to ask questions. TA will record how many times each student asks questions throughout the quarter. A student will get one tick letter grade bonus if she/he asks five or more questions by the end of the quarter.

- Class attendance is mandatory: you can miss no more than two lectures throughout the quarter. If you decide to show up, you have to arrive at the room no more than 5 min late. Late arrival will be treated as absence. If you miss three lectures, your letter grade will be reduced by one tick; if you miss five lectures, your letter grade will be reduced by two ticks; and so on.

- There is no final exam. However the final exam time may be used for presentations if we run out of presentation time.

- Grades will not be curved. The grading scheme here is designed to be as fair as possible and honor your efforts as accurately as possible. Most students did great in our class in the pass years.

**Suggested References**

Molecular Modelling by Leach; Covered chapters: 1, 4 - 9, 10, and 11. Students are encouraged to explore online for alternative reading materials.

**Lecture Outline**

- Review of biomolecules, biomolecular graphics, thermodynamics and molecular interactions, molecular mechanics, molecular dynamics and Monte Carlo, solvation and electrostatics, free energy and drug design.

- Biomolecular graphics using VMD will follow online tutorial at [http://www.ks.uiuc.edu/Training/Tutorials/vmd/tutorial-html/index.html](http://www.ks.uiuc.edu/Training/Tutorials/vmd/tutorial-html/index.html) The online tutorial will be left as homework to be finished by students at
home before student literature presentations. Note that use of VMD generated graphics in your presentation will boost your presentation scores.

• The instruction lectures will be complimented by presentations by distinguished outside speakers. There are four speakers lining up (all confirmed so far) for this quarter. The formal seminars will be joined by outside people not registered for the class AND WILL BE GIVEN IN A LARGER SEMINAR ROOM TO BE ANNOUNCED ONE WEEK AHEAD OF TIME. I will remind you before the seminar date so don’t go to the wrong room for these talks.

Class Logistics

• It is important to check email daily to make sure you don’t miss any announcements and assignments by email. Thus make sure your mailbox is not full and functions well throughout the quarter.

• Instructor’s presentation files and literatures will be posted on the class website before each lecture.

• For team presentations by undergraduates, each student is required to finish a draft powerpoint file 48 hours before the presentation time and email the file to the instructor. This is used as evidence that each student has independently reviewed the paper and prepared the presentation.

After the initial draft, the two students will need to work out the final presentation based on the two drafts before the presentation time. There are many ways to split the presentation by half and there is no restriction as long as each student presents roughly half of the materials.

After the presentation, all final presentations will need to be emailed to the instructor as record for final grade assignment.